2,3-Dibromothiophene 3140-93-0 | DTXSID80185324

Model Performance

Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 4.21e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.29e-01

Confidence level: 6.52e-01

Nearest Neighbors from the Training Set

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Benzothiophene Measured: 9.69e-04 Predicted: 6.71e-03

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Ethane, 1,2-diiodo-Measured: 6.06e-04 Predicted: 1.27e-03

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1,4-Dithiane

Measured: 2.50e-02 Predicted: 1.47e-02

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Benzothiazole Measured: 3.18e-02 Predicted: 2.15e-02

Image not found

Methylene iodide Measured: 4.63e-03 Predicted: 2.75e-03